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2-Propenoic Acid, Isodecyl Ester

(Isodecyl Acrylate; CAS RN 1330-61-6)

High Production Volume (HPV) Chemical Challenge: Final Test Status and Data Review

Prepared for:

ACC Specialty Acrylates and Methacrylates Panel

Prepared by:

Toxicology/Regulatory Services, Inc.

November 28, 2006

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Final Test Status

2-Propenoic Acid, Isodecyl Ester **(Isodecyl Acrylate; CAS RN: 1330-61-6)**		Information	OECD Study	GLP	Other Study	Estimation Method	Acceptable	Testing Required
STUDY		**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**
PHYSICAL AND CHEMICAL DATA								
2.1	Melting Point	Y	N	N	Y	Y	Y	N
2.2	Boiling Point	Y	N	N	Y	Y	Y	N
2.4	Vapor Pressure	Y	N	N	Y	Y	Y	N
2.5	Partition Coefficient	Y	N	N	N	Y	Y	N
2.6	Water Solubility	Y	N	N	Y	Y	Y	N
ENVIRONMENTAL FATE AND PATHWAY								
3.1.1	Photodegradation	Y	N	N	N	Y	Y	N
3.1.2	Stability in Water	Y	N	N	Y	N	Y	N
3.3	Transport and Distribution	Y	N	N	N	Y	Y	N
3.5	Biodegradation	Y	Y	N	N	N	Y	N
ECOTOXICITY								
4.1	Acute Toxicity to Fish	Y	Y	Y	N	Y	Y	N
4.2	Toxicity to Daphnia	Y	Y	Y	N	Y	Y	N
4.3	Acute Toxicity to Algae	Y	Y	Y	N	Y	Y	N
TOXICITY								
5.1	Acute Toxicity	Y	Y	Y	N	N	Y	N
5.4	Repeated Dose Toxicity	Y	Y	Y	N	N	Y	N
5.5	Genotoxicity *In Vitro* (Bacterial Test)	Y	Y	N	N	N	Y	N
5.5	Genotoxicity *In Vitro* (Mammalian Cells)	Y	Y	Y	N	N	Y	N
5.8	Reproductive Toxicity	Y	Y	Y	N	N	Y	N
5.9	Development Toxicity / Teratogenicity	Y	Y	Y	N	N	Y	N

2-Propenoic Acid, Isodecyl Ester (Isodecyl Acrylate; CAS RN 1330-61-6) High Production Volume Chemical Challenge: Final Test Status and Data Review

1.0 Introduction

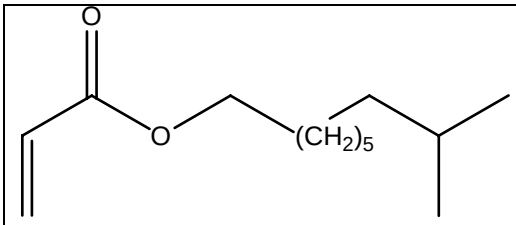
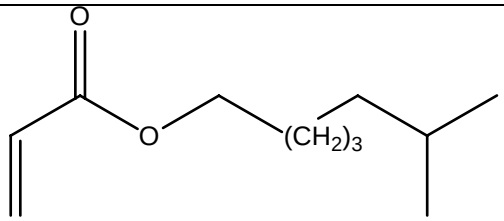
This document provides a Final Test Status and reviews the data for the High Production Volume (HPV) Chemical Challenge endpoints for 2-Propenoic Acid, Isodecyl Ester, hereafter called Isodecyl Acrylate [CAS RN 1330-61-6], for the ACC Specialty Acrylates and Methacrylates Panel.

2.0 General Use and Exposure

Isodecyl Acrylate is manufactured as an intermediate used for the synthesis of acrylic polymers. Applications include wood and vinyl coatings for floorings, pressure sensitive adhesives, paper coatings, release coatings, optical coatings and screen inks. Isodecyl Acrylate is used in ultraviolet and electron beam (UV/EB) processes for production of polymers. The UV/EB process is a low-energy technology that eliminates or greatly reduces the need for volatile organic solvents. In addition, the curing rate is very rapid and the reactions complete such that residual monomer is negligible in the final product. Occupational exposure may occur either as the liquid or vapor. Ventilation systems are used to limit vapor exposure. Air monitoring studies, reported in the SIAR for the closely related Isooctyl Acrylate (IOA), for processing and manufacturing areas have typically indicated airborne concentrations to be below the limit of detection. Since Isodecyl Acrylate is slightly less volatile than IOA, inhalation exposure of Isodecyl Acrylate to workers is not anticipated. Impermeable gloves are required to be worn by all employees who may come into contact with unreacted monomer. Based on the high cross-linking and very low residual monomer in finished products, consumer exposure to Isodecyl Acrylate is not anticipated.

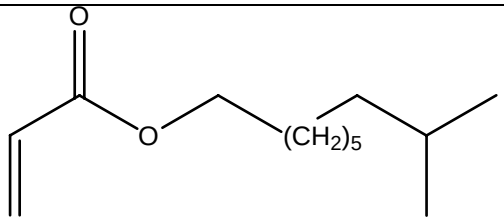
3.0 Justification for Use of Isooctyl Acrylate (IOA) Data to Support Isodecyl Acrylate

Isodecyl Acrylate and Isooctyl Acrylate, hereafter referred to as IOA, are very similar congeners of a large family of acrylic acid esters. They are comprised of long-chain hydrocarbon esters with terminal branching. Both chemicals are hydrophobic and similar in general physical/chemical and toxicological properties. The structures of these two acrylate esters are:

 Isodecyl Acrylate	 Isooctyl Acrylate (IOA)

A SIDS Assessment has been completed on IOA (SIDS, Volume 1, Part 2) and the key studies for the HPV Chemical Challenge endpoints are summarized in the IUCLID dossier for IOA that accompanies this Final Test Status and Data Review. The SIAM concluded: *"Based on its low occupational exposure potential, its low toxicity in in vitro and mammalian studies, its limited release to the environment and its predicted rapid environmental biodegradation, IOA is considered a low priority for additional human* health *or environmental effects testing at this time."* The physical/chemical properties, use patterns, potential environmental releases, and worker safety procedures are essentially the same for Isodecyl Acrylate and IOA. Therefore, the approach used in this HPV Chemical Challenge review document, in which IOA data are used extensively in support of the HPV/SIDS endpoints for Isodecyl Acrylate, is appropriate. Further, the above cited conclusions of the SIAM for IOA apply to Isodecyl Acrylate.

4.0 General Substance Information (Identity)

Chemical Name	2-Propenoic Acid, Isodecyl Ester
Synonyms	Acrylic acid, Isodecyl ester Isodecyl acrylate Isodecyl alcohol, acrylate Isodecyl propenoate
CAS Number	1330-61-6
Structure	
Molecular Weight	212.32
Substance Type	Organic
Physical State	Clear Liquid

5.0 Physical/Chemical Properties

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The Robust Summaries are included in the IUCLID Dataset. Although available data are provided below and in the IUCLID Dataset, it is not feasible to accurately measure the melting point for Isodecyl Acrylate, IOA, or other higher molecular weight acrylates or methacrylates at the very low temperatures required. Boiling of these monomers cannot occur in reality due to their rapid polymerization (see Boiling Point below) and, therefore, the boiling point can only be measured at reduced pressures. Subsequent extrapolation to standard pressure provides no useful information. Vapor pressure is intimately linked with boiling point and similarly cannot be measured at standard temperature and pressure. A detailed analysis of the physical/chemical properties of methacrylates (Jones, 2002) serves to illustrate this situation. In this study, physical/chemical properties of methacrylates from methacrylic acid to stearyl methacrylate were examined. Values for boiling point, vapor pressure, water solubility, and partition coefficient could not be measured or accurately extrapolated for methacrylate esters of greater than 8 carbons (e.g. octyl methacrylate). Although studies for similar acrylate esters are not available, the physical/chemical properties are similar and cannot be accurately determined for the higher molecular weight acrylate esters such as Isodecyl Acrylate and IOA.

5.1 Melting Point

The melting point for Isodecyl Acrylate from Handbook data (Lide, 1996) and from the Experimental Database for EPIWIN (U.S. EPA, 2005a) is -100ºC. No data were included in the accepted SIAR for IOA. The EPIWIN estimated melting point for Isodecyl Acrylate and IOA is 11.5 and -10.4 ºC, respectively. As noted above, accurate determination of melting point is not feasible and, therefore, these data are considered adequate to meet the HPV Chemical Challenge requirements.

5.2 Boiling Point

The boiling point for Isodecyl Acrylate from Handbook data (Lide, 1996) and from the Experimental Database for EPIWIN (U.S. EPA, 2005a) is 158 ºC. The boiling point accepted in the SIAR for IOA is 196.8 ºC (Xu and Vaishnav, 1992a). The EPIWIN estimated boiling point for Isodecyl Acrylate and IOA is 253.4 and 216.9ºC, respectively. The determination of the boiling point of IOA, Isodecyl Acrylate and other mono- and multi-functional acrylates is of minimal value. The double bond in these chemicals is so reactive that boiling them at atmospheric pressure results in polymerization and decomposition. As a result, these substances are not boiled at atmospheric pressure in normal manufacture or use. Moreover, distillation under vacuum at a lower temperature would generate a pure substance, since the inhibitor would be left behind. Without an inhibitor present, the pure substances quickly polymerize, even at room temperature. Therefore, the available data are considered adequate to meet the HPV Chemical Challenge requirements.

5.3 Vapor Pressure

The literature referenced (Howard and Meylan, 1997) and estimated model (U.S. EPA, 2005a) vapor pressure values for Isodecyl Acrylate at 25°C are 0.03 hPa and 0.02 hPa, respectively. The vapor pressure accepted in the SIAR for IOA is 1.33 hPa at 25 ºC (Xu and Vaishnav, 1992b) and the model predicts a vapor pressure of 0.15 hPa (U.S. EPA, 2005a). Although it is likely that the vapor pressure is actually lower, the value of 0.03 hPa is consistent with the large size and known properties of Isodecyl Acrylate. These data are considered adequate to meet the HPV Chemical Challenge requirements.

5.4 Partition Coefficient

The literature referenced (Howard and Meylan, 1997) and estimated model (U.S. EPA, 2005b) for the log K_{ow} value of Isodecyl Acrylate is 5.07 hPa. The log K_{ow} accepted in the SIAR for IOA is 3.93 (Method of Hunter *et al.*, 1985), and the model predicts a log K_{ow} value of 4.09 (U.S. EPA, 2005b). The value of 5.07 is consistent with the hydrophobicity and known properties of Isodecyl Acrylate. These data are considered adequate to meet the HPV Chemical Challenge requirements.

5.5 Water Solubility

As noted above, accurate measurement of water solubility for higher molecular weight acrylates is not readily accomplished. The reported value for water solubility of IOA that was accepted in the SIAR is 12.44 mg/L at 23.1ºC (Xu and Vaishnav, 1992c). The model estimated value (U.S. EPA, 2005c) for IOA is very similar, i.e. 16.9 mg/L. For Isodecyl Acrylate, the more hydrophobic ester group, isodecane, provides for a slightly lower water solubility. The literature referenced (Howard and Meylan, 1997) and model (U.S. EPA, 2005c) estimated values for water solubility of Isodecyl Acrylate of 1.75 mg/L and 12.14 mg/L, respectively, are consistent with the expectation of slightly lower solubility than IOA, as well as with the known properties of Isodecyl Acrylate. Jones (2002) was able to determine the water solubility for a C6 ester of methacrylate at 36 mg/L and a C8 ester at 7.8 mg/L, consistent with the information for the C8 acrylate, IOA. Therefore, although a measured value for Isodecyl Acrylate is not available, it is near 1 mg/L and the Handbook value, 1.75 mg/L, is considered adequate to meet the HPV Chemical Challenge requirements.

6.0 Environmental Fate

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The Robust Summaries are included in the IUCLID Dataset.

6.1 Photodegradation

The model prediction for atmospheric photodegradation of Isodecyl Acrylate provides a second order rate of reaction with hydroxyl radicals of 22.2 E-12 cm^3/molecule-sec and a half life ($t_{1/2}$) of 5.8 hours (U.S. EPA, 2005d). Similar values are estimated for IOA, 19.4 E-12 cm^3/molecule-sec and 6.6 hours, respectively. These data are considered adequate to meet the HPV Chemical Challenge requirements.

6.2 Stability in Water

Esters of acrylate and methacrylate are all hydrolytically stable at acidic and neutral pH. At approximately pH 11, these molecules rapidly hydrolyze (generally with $t_{1/2}$ of minutes) to acrylic acid and the appropriate alcohol. A broad database exists supporting this pH-dependent hydrolysis for these types of molecules, much of which has been submitted in the HPV Chemicals Challenge Program, the OECD SIDS program and others. The pH range relevant to determination of environmental fate is generally between pH 5 and 7. Therefore, hydrolysis is not a significant route of degradation in the environment and additional testing will not further the understanding of the environmental fate of Isodecyl Acrylate, particularly in light of the very low water solubility, making any effort to measure hydrolysis difficult. The model is not accurate for determination of hydrolysis but does 'recognize' the hydrolytic stability of the molecule indicating half lives of > 1 year at pH 7 and 8. Based on the extensive background data for acrylic and methacrylic esters, these data are considered adequate to meet the HPV Chemical Challenge requirements.

6.3 Transport and Distribution

Environmental exposure to Isodecyl Acrylate is limited based on the use patterns in UV/EB coating applications and the minimal residual monomer levels in final product polymers. Therefore, only accidental releases were considered for the fugacity modeling (U.S. EPA, 2005e). Two scenarios, 100% release to air and 100% release to water were examined. For the air release, the model predicted a distribution of 94% into atmosphere, 2.9% into water, 2.21% into soil, and 0.45% into sediment. Since there is uncertainty in the physical/chemical property values for Isodecyl Acrylate (i.e. they cannot be accurately measured), the fugacity model predictions were evaluated with water solubility and vapor pressures over two orders of magnitude. The following estimates resulted:

Water Solubility	**Vapor Pressure (mm Hg)**	**% in Air**	**% in Water**	**% in Soil**	**% in Sediment**
0.175	0.0227	94.4	2.9	2.2	0.5
1.75	0.0227	94.4	2.9	2.2	0.5
17.5	0.0227	94.4	2.9	2.2	0.5
1.75	0.0023	93.6	2.9	3.1	0.4
1.75	0.23	94.5	2.9	2.1	0.5

As clearly seen from the information in the table, the precision of the values for water solubility and vapor pressure is not critical for Isodecyl Acrylate because of the low solubility and vapor pressure.

For the water release, the model predicted a distribution of 2% into atmosphere, 85% into water, <0.1% into soil, and 13% into sediment. Similar estimates were made for IOA (U.S. EPA, 2005e). For 100% air release of IOA, the model predicted a distribution of 94.5% into atmosphere, 3% into water, 2% into soil, and 0.5% into sediment. For the water release, the model predicted a distribution of 2% into atmosphere, 85% into water, 0.5% into soil, and 13% into sediment. These data are considered adequate to meet the HPV Chemical Challenge requirements.

6.4 Biodegradability

As defined in the accepted SIAR, IOA has been shown to be rapidly degraded in an OECD 301D test (72% degradation in 5 days and 100% degradation in 28 days) and is readily biodegradable (3M, unpublished data). The similar structure of Isodecyl Acrylate indicates that it will also undergo rapid biodegradation in the environment. In addition, the closely related, Isodecyl Methacrylate (submitted in the Hydrophobic Methacrylate Category for ICCA), degraded 88% in 28 days although the 10-day window was not met (Elf Atochem, 2001). These data are considered adequate to meet the HPV Chemical Challenge requirements.

7.0 Ecotoxicity

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The Robust Summaries are included in the IUCLID Dataset.

7.1 Toxicity to Fish

The 96-hour LC_{50} value for the fathead minnow accepted for IOA in the SIAR is 0.67 mg/L (Amato and Vaishnav, 1992a). Although the estimated water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Chemical Challenge program and indicates that Isodecyl Acrylate is toxic to fish.

7.2 Toxicity to Aquatic Invertebrates

The 48-hour EC_{50} value for *Daphnia magna* accepted for IOA in the SIAR is 0.4 mg/L (Amato and Vaishnav, 1992b). Although the estimated water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Chemical Challenge program and indicates that Isodecyl Acrylate is toxic to aquatic invertebrates.

7.3 Toxicity to Aquatic Plants

The 96-hour E_rC_{50} value for algae accepted for IOA in the SIAR is 2.13 mg/L (Vaishnav, 1992). The NOEC was 1.70 mg/L. Although the water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Chemical Challenge program and indicates that Isodecyl Acrylate is toxic to aquatic invertebrates.

7.4 Chronic Toxicity to Aquatic Invertebrates

IOA was tested in a reproduction study with *Daphnia magna* that was accepted as part of the SIAR review. The 21-day survival and reproduction were reported. Based on the mean measured concentrations, the 21-day EC_{50} and IC_{50} values for survival and reproduction were 1.61 and 1.02 mg/L, respectively, and the 21-day NOECs were 1.06 mg/L and < 0.20 mg/L, respectively. The 14-day survival and reproduction toxicity were also determined. Based on the mean measured concentrations, the 14-day EC_{50} and IC_{50} values were 1.99 mg/L and 0.97 mg/L, respectively, and the 14-day NOECs for survival and reproduction were 1.09 mg/L and 0.51 mg/L, respectively. These values confirmed that IOA and Isodecyl Acrylate, by analogy, are toxic to aquatic invertebrates (Amato and Mount,1993).

8.0 Human Health-Related Data

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The Robust Summaries are included in the IUCLID Dataset. These studies are all for IOA.

8.1 Acute Toxicity

The acute oral LD_{50} in rats for IOA accepted for the SIAR is > 5000 mg/kg body weight (Glaza, 1989; Gordon *et al.*, 1991). This value is consistent with the limited toxicity of hydrophobic acrylate and methacrylate esters and is considered appropriate for Isodecyl Acrylate. These data are considered adequate to meet the HPV Chemical Challenge requirements.

8.2 Repeated Dose Toxicity

IOA was tested using the OECD 422 Combined Repeat Dose and Reproductive/ Developmental Screening Test (Henwood, 1993) that was accepted for the SIAR. In this test, male and female Fischer 344 rats were treated with 0%, 1.0%, 7.5%, 15%, or 25% (lowered to 20% after one week) IOA in acetone at a dose volume of 100 µL/day for at least six hours/day for two weeks prior to breeding and during breeding, gestation, and through postnatal day 4. Dermal irritation, consisting of slight to moderate erythema, slight to moderate desquamation, and slight fissuring (females only) was observed in the high dose group. Slight increases in serum aspartate aminotransferase and alanine aminotransferase concentrations were noted in males from the high dose group. No other treatment-related effects were observed and the NOAEL was 15% in the diet. Based on the very limited systemic effects in this study and recognizing that the primary route of potential exposure to Isodecyl Acrylate is via skin contact, these data are adequate to support the conclusion that no significant toxicity is anticipated from dermal exposure to Isodecyl Acrylate. Therefore, the available data are considered adequate to meet the HPV Chemical Challenge requirements.

8.3 Genetic Toxicity

8.3.1 *In vitro*

IOA was tested in a bacterial gene mutation assay according to OECD Guideline 471 with *Salmonella* strains TA1535, TA1537, TA1538, TA98 and TA100. IOA was negative with and without metabolic activation at concentrations ranging from 0.005 to 0.5 µL/plate (Mortelmans and Pomeroy, 1980; Gordon *et al.*, 1991).

IOA was tested in a mouse lymphoma assay according to OECD Guideline 476. There was no evidence of mutagenicity in this mammalian cell assay at concentrations ranging from 0.0015 to 0.11 µL/plate (Kirby, 1980; Gordon *et al.*, 1991).

Isodecyl Acrylate and IOA are members of a large family of acrylic acid esters. A large battery of mutagenicity screening tests exists for these chemicals and the results of these studies have been submitted in other HPV and SIDS Dossiers. These include lower molecular weight acrylate esters which would be much more readily taken up by bacterial and mammalian cells than the larger IOA and Isodecyl Acrylate esters. In some cases, extensive testing has been conducted; e.g. ethyl acrylate. In some assays, ethyl acrylate

resulted in a positive response. However, in all of these studies, positive results occurred only at concentrations that led to a clearly reduced cell survival rate, and the increase in the number of mutants while dose-dependent, did not attain a doubling in mutant frequency in cultures showing at least 50% relative total growth. Other acrylate esters that have been evaluated in similar assays and were shown to form small colony mutants indicative of chromosomal aberrations (Moore and Doerr, 1990, and references cited therein). More recent studies indicated that there is an association between chromosomal aberrations and cytotoxicity at exposure concentrations which reduce cell growth to less than 50% of the control value (Galloway, 2000, and references cited therein). These data suggest that the increase in mutagenicity reported in the gene mutation assays with acrylates are an artifact of the experimental method. Overall, the conclusion that acrylate esters are not mutagenic *in vivo* has been consistent across the family. Of particular note, is the tendency for positive responses to be observed in mouse lymphoma cells. As noted above, IOA was negative in both bacterial and mammalian cell systems, specifically mouse lymphoma cells. This is consistent with the conclusion that these esters are not mutagenic. Further, the SIAR for IOA concluded that the exposure and low toxicity of these chemicals indicates that further testing will not provide additional knowledge of the potential hazards. Since there are no significant toxicological differences observed for IOA and Isodecyl Acrylate,, the available data are considered adequate to meet the HPV Chemical Challenge requirements, consistent with the IOA SIAR.

8.4 Reproductive and Developmental Toxicity

IOA was tested using the OECD 422 Combined Repeat Dose and Reproductive/ Developmental Screening Test (Henwood, 1993) that was accepted for the SIAR. In this test, male and female Fischer 344 rats were treated with 0%, 1.0%, 7.5%, 15%, or 25% (lowered to 20% after one week) IOA in acetone at a dose volume of 100 µL/day for at least six hours/day for two weeks prior to breeding and during breeding, gestation, and through postnatal day 4 (see Repeated Dose Toxicity above). There were no treatment-related effects on male fertility, female fertility, mean days to mating, length of gestation, pup viability, mean number of pups/litter, or pup weights. There were no treatment-related findings at necropsy of the pups. Reproductive organ weight and histopathology findings for the adults were similar to controls. The reproductive and developmental NOAEL was 20%. Based on the lack of effects in this study and recognizing that the primary route of potential exposure to Isodecyl Acrylate is via skin contact, these data are adequate to support the conclusion that no reproductive or developmental toxicity is anticipated from exposure to Isodecyl Acrylate. Therefore, the available data are considered adequate to meet the HPV Chemical Challenge requirements.

9.0 Conclusion

Isodecyl Acrylate and IOA are very similar congeners of a large family of acrylic acid esters. Therefore, the data for IOA have been used extensively in evaluation of the HPV/SIDS endpoints for Isodecyl Acrylate. Adequate information is available for melting point, boiling point, vapor pressure, water solubility and partition coefficient for both chemicals. Photodegradation and environmental distributions are adequately supported by the appropriate

model data for Isodecyl Acrylate and the model data for IOA support the similarity of the chemicals. Hydrolysis of acrylic acid esters does not occur at physiological or environmental pH. The aquatic tests with fish, invertebrates and plants for IOA indicate that IOA, Isodecyl Acrylate and other hydrophobic acrylic esters are toxic to aquatic organisms. Since IOA (and therefore, Isodecyl Acrylate) rapidly biodegrades in the environment and environmental exposure is limited, the degradation and toxicity studies for IOA are adequate to support Isodecyl Acrylate environmental fate and effects. The oral LD50 of IOA is > 5000 mg/kg and subchronic toxicity evaluations indicate that only skin irritation would be anticipated from exposure to these hydrophobic acrylate esters. IOA is not mutagenic in screening assays consistent with the family of acrylic acid esters. Isodecyl Acrylate, therefore, is also considered not to pose a mutagenic hazard. As with repeated dose toxicity, evaluation of the reproductive and developmental toxicity of IOA is adequate for Isodecyl Acrylate and indicates that Isodecyl Acrylate does not affect reproduction or the developing offspring. Overall, the available data for IOA, consistent with the conclusions of the SIAM, are considered adequate to meet the HPV Chemical Challenge Program requirements and serve to similarly support Isodecyl Acrylate.

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Table 1: Data Summary

2-Propenoic Acid, Isodecyl Ester

CAS NO: 1330-61-6		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point		Handbook Data – for Isodecyl Acrylate	-100 ºC
2.2	Boiling Point		Handbook Data – for Isodecyl Acrylate	158 ºC
2.4	Vapor Pressure		Handbook Data – for Isodecyl Acrylate	0.03 hPa (at 20 ºC)
2.5	Partition Coefficient (log K_{ow})		KOWWIN v. 1.67 – for Isodecyl Acrylate	5.07
2.6	Water Solubility		Handbook Data – for Isodecyl Acrylate	1.75 mg/L
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		AOPWIN v. 1.91 – for Isodecyl Acrylate	Half-life: 5.8 hours (OH Rate Constant: 22.2 E-12 cm^3/molecule-sec)
3.1.2	Stability in Water			Acrylate esters are stable at pH 3 and 7 and hydrolyze rapidly to acrylate and the associated alkyl chain alcohol at pH 11.
3.3	Transport and Distribution		Mackay Level III: – for Isodecyl Acrylate 100% release to air	94% into atmosphere, 2.9% into water, 2.2% into soil, 0.5% into sediment
			– for Isodecyl Acrylate 100% release to water	2% into atmosphere, 85% into water, <0.1% into soil, 13% into sediment
3.5	Biodegradation		OECD 301D – for IOA	100% after 28 days; Readily Biodegradable
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Pimephales promelas*	OECD 203 – for IOA	LC_{50} (96 hours) = 0.67 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates	*Daphnia magna*	OECD 202 – for IOA	EC_{50} (48 hours) = 0.4 mg/L
4.3	Toxicity to Aquatic Plants e.g. Algae	Green algae	OECD 201 – for IOA	E_rC_{50} (72 hours) = 2.13 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	*Daphnia magna*	OECD 202 – for IOA	14-Day IC_{50} (Reproduction) = 0.97 mg/L 21-Day IC_{50} (Reproduction) = 1.02 mg/L

Table 1: Data Summary

2-Propenoic Acid, Isodecyl Ester

CAS NO: 1330-61-6		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY				
5.1	Acute Oral Toxicity	Rat	OECD 401 – for IOA	LD_{50} : >5000 mg/kg bw
5.7	Repeated Dose Toxicity	Rat - Dermal	OECD 422 – for IOA	NOAEL = 15% (100 µl/day)
5.8	Genetic Toxicity *In Vitro*			
	Bacterial Test (Gene mutation)	*Salmonella typhimurium*	OECD 471 – for IOA	Negative
		Mouse lymphoma	OECD 476 – for IOA	Negative
5.11	Toxicity to Reproduction / Impairment of Fertility	Rat - Dermal	OECD 422 – for IOA	NOAEL = 20% (100 µl/day)
5.12	Developmental Toxicity / Teratogenicity	Rat - Dermal	OECD 422 – for IOA	NOAEL = 20% (100 µl/day)

IOA = Isooctyl Acrylate